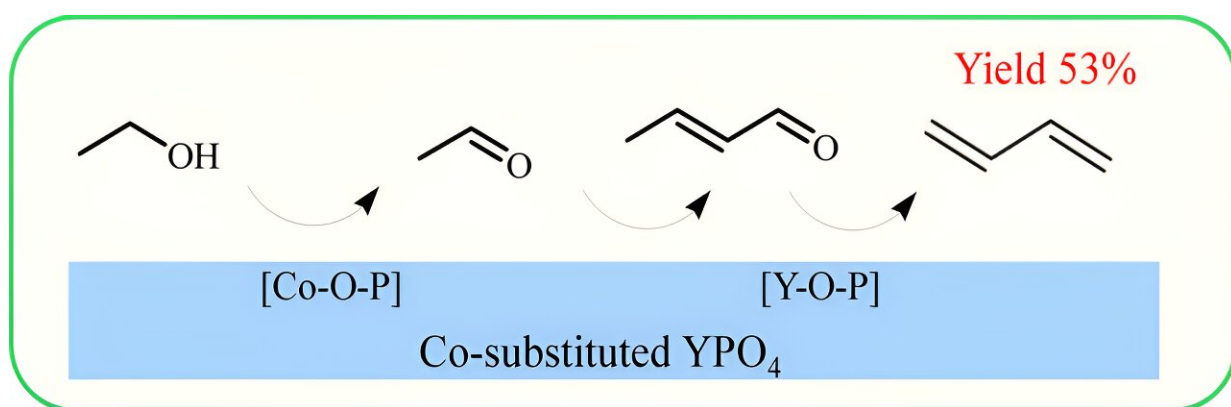


# Strong coordination interaction identified as being favorable for promoting ethanol dehydrogenation

March 13 2024



A strong coordination interaction between Co<sup>2+</sup> sites and PO<sub>4</sub><sup>3-</sup> on YPO<sub>4</sub> has been identified, being favorable for promoting ethanol dehydrogenation. Rare-earth Y<sup>3+</sup> cations stabilized by phosphates serve as robust Lewis acid catalysts for C–C coupling reaction. Credit: Chinese Journal of Catalysis

Butadiene, one of the most important light olefins in the petrochemical industry with a global production capacity of 18 million metric tons per year, is currently produced through the extractive distillation of C<sub>4</sub> fractions from naphtha steam cracking processes or dehydrogenation of C<sub>4</sub> hydrocarbons, both of which involve extensive energy consumption and significant emission of CO<sub>2</sub>.

The increasing market demand has raised much interest in on-purpose production of these feedstocks. Thus, an [alternative route](#) to directly produce butadiene using any sustainable feedstocks is desirable and prospective.

Ethanol, as a carbon-neutral resource, can in principle undergo C-C bond formation to yield butadiene sustainably. Traditional catalytic systems have been classified into two categories: group 4 and 5 [transition metals](#), and MgO-SiO<sub>2</sub>.

Among reported catalysts, Zn-Y/Beta is particularly noteworthy owing to its good selectivity for butadiene (>60%). Although great efforts were put into this direction, the steady production of butadiene from ethanol under mild reaction conditions remains an unsolved challenge, generally leading to quick deactivation. Another difficulty for butadiene formation is that the dehydration often competes with dehydrogenation reaction over Lewis acidic [catalyst](#).

A research team led by Prof. An-Hui Lu from Dalian University of Technology, China, has reported the first cobalt-doped yttrium phosphate (Co-YPO<sub>4</sub>) catalyst, for preferential activation of ethanol to form acetaldehyde and subsequent C-C coupling and dehydration to butadiene. The catalyst exhibited 68.5% selectivity to butadiene in an ethanol conversion of 78.2% at 350 °C, and thereby close to 61% yield to total olefin (butadiene and ethene). The work is [published](#) in the *Chinese Journal of Catalysis*.

Combined with various in situ characterizations, a strong coordination interaction between Co<sup>2+</sup> sites and the phosphate group on YPO<sub>4</sub> has been identified as being favorable for improving ethanol dehydrogenation performance.

The YPO<sub>4</sub> surface exposed the Y<sup>3+</sup> site, which can effectively catalyze

the C-C coupling reaction. Through the combination of the Co and Y species in one catalyst, i.e. Co-YPO<sub>4</sub>, the synergistic effect of the bifunctional sites could be achieved.

**More information:** Bai-Chuan Zhou et al, PO<sub>4</sub><sup>3-</sup> coordinated Co<sup>2+</sup> species on yttrium phosphate boosting the valorization of ethanol to butadiene, *Chinese Journal of Catalysis* (2024). [DOI: 10.1016/S1872-2067\(23\)64567-X](https://doi.org/10.1016/S1872-2067(23)64567-X)

Provided by Chinese Academy of Sciences

Citation: Strong coordination interaction identified as being favorable for promoting ethanol dehydrogenation (2024, March 13) retrieved 27 April 2024 from <https://phys.org/news/2024-03-strong-interaction-favorable-ethanol-dehydrogenation.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.